

# Creep in Zirconium Described with Fully Atomistic Simulations Coupled to VPSC Models

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Zirconium is the most widely used element for cladding material in pressurized water reactors. The cladding is the last confinement barrier that prevents unstable atom release and is susceptible to creep under the influence of internal pressure and temperature due to residual fuel power and radiation. Atomistic simulations are used to observe phenomena, such as diffusion and aggregation of interstitials and vacancies, and parameterize the Visco Plastic Self Consistent (VPSC) model, which describes creep at experimentally relevant length and time scales.

Creep is a time-dependent irreversible deformation that occurs at a low rate and at stresses below the ultimate stress of the material. Non-hydrostatic stresses (i.e., shear stresses) are required for creep. Two different kinds of creep are relevant in cladding materials, namely thermal creep and irradiation creep. Both these deformation processes require elevated temperatures and applied stresses, while the latter also requires the presence of irradiation.

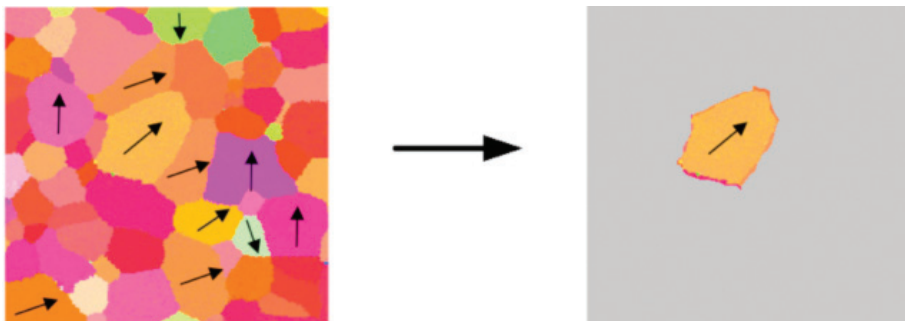
The Visco-Plastic Self Consistent (VPSC) model [1] describes creep on the grain level (micron scale), by treating each grain as if it is immersed in an effective medium. This model is attractive because of its predictive capability over experimentally relevant time and length scales. It can provide useful design guidelines, direct experiments, and aid in the phenomenological interpretation of measurements. However, parameterizing VPSC requires a large amount of non-trivial information about the system. Traditionally, either of two approaches has been employed: 1) greatly simplified models of physically relevant systems are used to extract these parameters, or 2) parameters are fit to

experimental data. As a result, descriptions of creep are usually valid only in a limited range of conditions, with severely restricted predictive capability.

In the present work, we use state-of-the-art accelerated molecular dynamics (AMD) simulation methodologies developed at LANL to significantly extend the time scales accessible by direct fully-atomistic simulations. These lead up to a complete parameterization of a VPSC description of the system that contains no adjustable parameters. This enables us to assess the prevalence of various mechanisms that contribute to creep, and the accuracy of different theories. We chose to study zirconium (Zr) in particular because of its relevance to LANL missions and its industrial prevalence.

VPSC models of creep in Zr require the rate at which point defects (interstitials, vacancies) are absorbed by line defects (dislocations, dislocation loops, and vacancy loops). We use existing Zr potentials [2], developed using Density Functional Theory (DFT), to characterize the dynamical processes that lead to defect absorption by line defects. This involves mapping out various interconversion and diffusion processes that point defects can undergo, and the energy barriers associated with them, as these determine the diffusive behavior of defects. The effect of strains (either external, or due to the presence of line defects) on these interconversion rates is incorporated by computing dipole tensors. These dipole tensors are a characteristic property of a defect and describe the energy gained by the defect in the presence of a strain field. Figure 2 shows the energy landscape of an interstitial in the strain field of an edge dislocation. We use molecular statics to compute dipole tensors, and molecular dynamics (MD) and AMD to discover

Fig. 1. Schematic of the principle behind VPSC. The deformation of a single grain is computed by replacing the surrounding grains by an effective medium. This process is repeated for all grains in the system.



and characterize interconversion processes. In particular, we use Temperature Accelerated Dynamics (TAD) [3]—a specialized method that is built upon Harmonic Transition State Theory (HTST). TAD involves running MD at elevated temperatures, and extrapolating the results to lower temperatures. This results in the system exploring the potential energy surface orders of magnitude faster than it would have otherwise done, without loss of atomistic detail. We also characterize defect interconversion rates by computing the energy barriers and prefactors associated with each transition [4]. The catalog of events and barriers thus obtained will be fed into a Kinetic Monte Carlo simulation, to compute the net absorption rate of point defects by a variety of line defects. These rates will be used to compute dislocation climb rates, which form part of the parameterization of the VPSC description of creep.

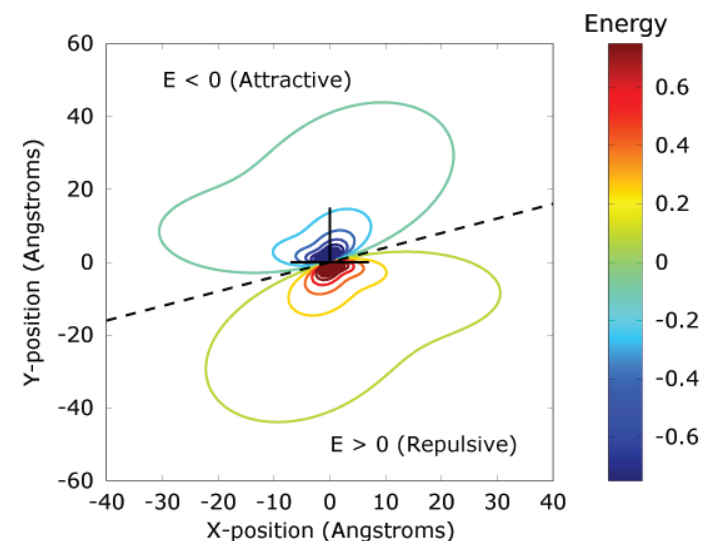


Fig. 2. Energy landscape of an interstitial due to the strain field around an edge dislocation. One side of the dislocation attracts interstitials, while the other repels them.

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